2-Ethyl-p-xylene 1758-88-9 | DTXSID0061951

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: -63.5 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 7.66e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Dimethyl-4-ethylbenzene

Measured: -62.9 **Predicted:** -63.5

Image not found

1,2-Dimethyl-4-ethylbenzene

Measured: -66.9 **Predicted:** -63.5

Image not found

2-Ethyl-p-xylene Measured: -53.7 Predicted: -63.5

Image not found

1-Ethyl-2,3-dimethylbenzene

Measured: -49.5 Predicted: -63.5

Image not found

1,3-Dimethyl-5-ethylbenzene

Measured: -84.3 Predicted: -63.5